August 20, 2003

Frederick R. Johannsen
Technical Contact
Solutia, Inc.
575 Maryville Centre Drive
St. Louis, MI 63141

Dear Mr. Johannsen:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for 4-Nitrophenol posted on the ChemRTK HPV Challenge Program Web site on April 17, 2003. I commend Solutia, Inc. for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed Comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that Solutia, Inc. advise the Agency, within 60 days of this posting on the Web site, of any modifications to its submission. Please send any electronic revisions or comments to the following e-mail addresses: oppt.ncic@epa.gov and chem.rtk@epa.gov.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-*S*-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: W. Penberthy
M. E. Weber

EPA Comments on Chemical RTK HPV Challenge Submission:
4-Nitrophenol

Summary of EPA Comments

The sponsor, Solutia, Inc., submitted a test plan and robust summaries to EPA for 4-Nitrophenol (PNP; CAS No. 100-02-7) dated April 9, 2003. EPA posted the submission on the ChemRTK HPV Challenge Web site on April 17, 2003.

EPA has reviewed this submission and has reached the following conclusions:

1. Physicochemical Properties. The data provided by the submitter for melting point, octanol/water partition coefficient and water solubility are adequate for the purposes of the HPV Challenge Program. The submitter needs to re-examine the boiling point and vapor pressure data.

2. Environmental Fate. The submitter needs to address some deficiencies and errors for photodegradation, biodegradation, and fugacity. The submitter needs to incorporate hydrolysis information in robust summary format.

3. Health Effects. Adequate data are available for acute, repeated-dose, genetic, and reproductive toxicity endpoints for the purposes of the HPV Challenge Program. The submitter needs to provide additional information for developmental toxicity.

4. Ecological Effects. Available data are adequate for the purposes of the HPV Challenge Program.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

EPA Comments on the 4-Nitrophenol Challenge Submission

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient and water solubility)

The data provided by the submitter for melting point, octanol/water partition coefficient and water solubility are adequate for the purposes of the HPV Challenge Program.

Boiling point. The boiling point for 4-nitrophenol is given as >279 °C in Table 2 on page 9; however, according to handbook sources this value reflects decomposition (Verschuren, K. 2001. Handbook of environmental data on organic chemicals, 4th ed. New York, NY: John Wiley & Sons, p. 1636). The submitter needs to state that this is a decomposition temperature.

Vapor pressure. The submitter obtained a calculated vapor pressure of 0.0067 hPa (0.0050 mmHg) at 20 °C from HSDB 2002. However, the value for PNP from Schwarzenbach et al. (1988) was misreported in the HSDB. The value 0.0050 mmHg corresponds to the vapor pressure at 20 °C for the subcooled liquid of 2,4-dinitrophenol.

Schwarzenbach et al. also reported extrapolated vapor pressures for 4-nitrophenol at 20 °C of 1.10×10^{-6} atm (8.33×10^{-4} mmHg) for the subcooled liquid, and 1.29×10^{-7} atm (9.79×10^{-5} mmHg) for the solid. The value for solid 4-nitrophenol can satisfy the endpoint in this case.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity)

Adequate data are available for these endpoints for the purposes of the HPV Challenge Program.

Photodegradation. The submitter provided values of 5.7 days (pH 5), 6.7 days (pH 7), and 13.7 days (pH 9) (Hustert et al. 1981). The submitter indicates that these values compare favorably with an AOPWIN estimated value of 2.48 days based on a 12-hr day and 1.5 x 10^6 OH/cm^3. This comparison is in error. The data in Hustert et al. (1981) are for direct photolysis in aqueous solution by sunlight. The estimations from AOPWIN provide half-lives for the reactions of vapor phase 4-nitrophenol with photochemically generated hydroxyl radicals. The submitter needs to address this error.

Stability in water. While EPA agrees that this chemical is stable to hydrolysis, the submitter needs to include this information in a robust summary. Furthermore, the submitter needs to indicate that 4-nitrophenol does degrade in water upon exposure to sunlight, referencing the relevant data presented in the photodegradation section.

Biodegradation. The submitter needs to provide a detailed description of each test including the OECD Screening test, and resolve other issues identified under the comments on the robust summaries.

Fugacity. The submitter used an incorrect vapor pressure in the input parameters. The correct value for 4-nitrophenol is 9.79x10^{-5} mmHg (see vapor pressure section, above). The submitter's Henry's law constant is not consistent with the experimental value cited in the PHYSPROP database, 4.15x^{-10} atm-m^3/mole (Parsons et al. 1971). The submitter used half-lives in air, water, soil, and sediment that were very short, and did not explain why these were used. The submitter needs to address these vapor pressure, Henry's law constant, and half-life input issues.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity)

Adequate data are available for acute, repeated-dose, genetic, and reproductive toxicity endpoints for the purposes of the HPV Challenge Program. The submitter needs to provide additional information for the developmental toxicity endpoint.

Repeated-dose toxicity. The submitter needs to include in the robust summaries the 18-month chronic toxicity study in mice (NTP, 1994) discussed in the test plan.

Genetic toxicity (gene mutation). The submitter needs to provide separate robust summaries for the *Drosophila* sex-linked recessive lethal assay (NTP, 1994) and the NTP's CHO-HGPRT forward mutation assay (Oberly et al, 1990), which are discussed as supporting data in the test plan.

Genetic toxicity (chromosomal aberration). The submitter needs to provide the SCE assay as a separate robust summary.

Developmental toxicity. The submitter needs to discuss the developmental toxicity criteria for the submitted 2-generation reproductive toxicity study. Since the study was conducted with much lower doses than those recommended by the OECD guidelines for the dermal route, and did not elicit any maternal toxicity at the highest dose tested, the submitter needs to provide information on the selection of doses and exposure route.

The test plan and Tables 1 and 5 in the test plan need to specifically address the developmental toxicity endpoint.

Ecological Effects (fish, invertebrates, and algae)

The studies submitted on fish, invertebrates and algae adequately address these endpoints.

Specific Comments on the Robust Summaries

Generic Comments

Some of the definitive values (*e.g.,* EC50/LC50 and NOAELs/LOAELs) were reported as greater than or equal to (≥) in the respective fields. The submitter needs to remove the greater than (>) sign.

Environmental Fate

Biodegradation. (a) The submitter indicates that it used five OECD guideline 301 methods. However, the only tests that seem to follow OECD Guideline 301 are the Sturm test (301 B), the OECD Screen test (301 E), and the Closed Bottle test (301 D). This point needs clarification. (b) The Zahn-Wellens test is OECD Guideline 302 B for determining inherent biodegradability, not ready biodegradation as indicated in the robust summary. (c) The submitter needs to indicate clearly and accurately which tests provide inherent biodegradation results and which provide ready biodegradation results, rather than categorize them all as ready biodegradation. (d) The degradation time periods for the MITI test, the AFNOR test, and the Sturm test are missing.

Ecological Effects

Algae. The submitter needs to provide the test concentrations used in the algal study.

Followup Activity

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.